



```

chain nodes :
  7 9 16 29 34 35 73
ring nodes :
  1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22 23 24 25 26 27 28 37
  38 39 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65
  66 67
chain bonds :
  1-34 4-35 7-9 7-14 16-21 27-29 35-73
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-37 6-39 10-11 10-15 11-12 12-13 13-14 14-15 17-18
  17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 37-38 38-39
  44-45 44-49 45-46 46-47 47-48 48-49 50-51 50-55 51-52 52-53 53-54 54-55 56-57
  56-61 57-58 58-59 59-60 60-61 62-63 62-67 63-64 64-65 65-66 66-67
exact/norm bonds :
  1-34 4-35 5-37 6-39 7-9 7-14 10-11 10-15 11-12 12-13 13-14 14-15 16-21 17-18
  17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 27-29 35-73
  37-38 38-39
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 44-45 44-49 45-46 46-47 47-48 48-49 50-51 50-55 51-52
  52-53 53-54 54-55 56-57 56-61 57-58 58-59 59-60 60-61 62-63 62-67 63-64 64-65
  65-66 66-67

```

G2:O,S,N

G3:[*1],[*2],[*3]

G4:C,S,N

G5:C,N

G6:Cb,[*4],[*5],[*6],[*7]

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom
13:Atom

```

	14:Atom	15:Atom	16:CLASS	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	22:Atom
23:Atom	24:Atom	25:Atom	26:Atom	27:Atom	28:Atom	29:CLASS	34:CLASS	35:CLASS	37:Atom
38:Atom	39:Atom	44:Atom	45:Atom	46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom
52:Atom	53:Atom	54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom
62:Atom	63:Atom	64:Atom	65:Atom	66:Atom	67:Atom	73:CLASS			